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From clean to diffusive mesoscopic systems: A semiclassical approach to the magnetic susceptibility

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Abstract. – We study disorder-induced spectral correlations and their effect on the magnetic susceptibility of mesoscopic quantum systems in the non-diffusive regime. By combining a diagrammatic perturbative approach with semiclassical techniques we perform impurity averaging for non-translational invariant systems. This allows us to study the crossover from clean to diffusive systems. As an application we consider the susceptibility of non-interacting electrons in a ballistic microstructure in the presence of weak disorder. We present numerical results for a square billiard and approximate analytic results for generic chaotic geometries. We show that for the elastic mean free path ℓ larger than the system size, there are two distinct regimes of behaviour depending on the relative magnitudes of ℓ and an inelastic scattering length.

Phase-coherent, disordered conductors where the electron motion equals a random walk between impurities have traditionally been of interest in mesoscopic physics [1]. Random walks occur in the diffusive regime where the elastic mean free path ℓ is much smaller than the system size L . On the other hand, the development of high-mobility semiconductor heterostructures, combined with advanced lithographic techniques, have allowed the confinement of electrons to two-dimensional microstructures of controllable, non-random geometry. They have been coined “ballistic” since $\ell > L$. Nevertheless, residual impurity scattering is nearly unavoidable even in these systems and it became clear that disorder can be strong enough to mix energy levels and effect the two-level correlation function, $K(\varepsilon_1, \varepsilon_2)$, even in the “ballistic” regime [2, 3]. There it is necessary to consider both disorder averaging, $\langle \dots \rangle_d$, and size (or energy) averaging, $\langle \dots \rangle_L$. After such averaging the two-level correlation function may be divided into two separate terms [3], $\langle K^d(\varepsilon_1, \varepsilon_2) \rangle_L = \langle \langle \nu(\varepsilon_1) \nu(\varepsilon_2) \rangle_d \rangle_L - \langle \langle \nu(\varepsilon_1) \rangle_d \langle \nu(\varepsilon_2) \rangle_d \rangle_L$ and $K^L(\varepsilon_1, \varepsilon_2) = \langle \langle \nu(\varepsilon_1) \rangle_d \langle \nu(\varepsilon_2) \rangle_d \rangle_L - \bar{\nu}^2$, where ν denotes the single particle density of states and $\bar{\nu} = \langle \langle \nu(\varepsilon) \rangle_d \rangle_L$ its mean part. K^d is a measure of *disorder-induced* correlations of ν , while K^L is given by *size-induced* correlations.

The orbital magnetism of isolated mesoscopic systems has been the subject of much theoretical interest, in particular because it is sensitive to spectral correlations: For a system with

a fixed number of particles it is necessary to consider averaging under canonical conditions [4, 5, 6] resulting in a large contribution to the average magnetism. The corresponding susceptibility is given by [6] $\langle \chi(H) \rangle = -(\Delta/2) \partial^2 / \partial H^2 \langle \delta N^2(\mu; H) \rangle$. Here H is the magnetic field, Δ is the mean level spacing and $\langle \delta N^2(\mu; H) \rangle$ is the variance in the number of energy levels within an energy interval of width equal to the chemical potential, μ . This variance is related to $K(\varepsilon_1, \varepsilon_2; H)$ by integration of the level energies $\varepsilon_1, \varepsilon_2$ over the energy interval. In the following we will label the contributions to the susceptibility, corresponding to $\langle K^d \rangle_L$ and K^L , as $\langle \chi^d(H) \rangle$ and $\langle \chi^L(H) \rangle$, respectively, so that $\langle \chi(H) \rangle = \langle \chi^d(H) \rangle + \langle \chi^L(H) \rangle$.

For real systems, besides ℓ , there are additional relevant lengthscales at which inelastic scattering (L_ϕ) or temperature smearing (L_T) produce a damping of propagation. For clarity we refer to such a lengthscale as L_ϕ , although we assume that similar general arguments will hold for finite L_T . For ballistic motion, L_ϕ is related to the level broadening γ by

$$\frac{L_\phi}{L} = \frac{k_F L}{2\pi} \frac{\Delta}{\gamma} \quad (1)$$

with k_F being the Fermi momentum. It divides the “ballistic” regime into two sub-regimes. In the first, $L, L_\phi < \ell$, the particle motion is nearly ballistic since damping due to inelastic scattering typically occurs before impurity scattering; for the remainder of this paper we refer to this regime as *inelastic*. In the second, $L < \ell < L_\phi$, a particle may scatter many times off impurities before scattering inelastically and we refer to this regime as *elastic*.

In this paper we employ a systematic semiclassical approach to calculate the contribution of orbits of *all lengths* in the elastic and inelastic regimes to weak field $\langle \chi^d(H) \rangle$ for microstructures with white noise disorder [7]. Energy and impurity averaging are performed within a diagrammatic perturbation approach applicable to the “ballistic” regime. In contrast to many techniques valid for bulk disordered systems, $\ell < L$, we do not assume translational invariance. Instead, we use an approach related to the “method of trajectories” devised for thin superconducting films [8] and we write Green functions semiclassically in terms of classical paths which include the effect of boundary scattering. Note that similar [9], and alternative [10], methods have been used to consider weak localization in thin films in a parallel magnetic field. Our approach allows us to study the complete crossover from diffusive to clean systems for arbitrary values of L_ϕ (smaller than $v_F t_H$, where t_H is the Heisenberg time). We present results for ballistic systems with both chaotic and integrable dynamics in the clean limit. As an example of an integrable geometry, we treat the case of the square billiard. Experiments [11] on the orbital magnetism of ensembles of squares were performed in the “ballistic” (inelastic) regime, motivating theoretical studies of the susceptibility for $L < \ell$ [12, 13].

Semiclassical diagrammatic approach. – We begin by presenting some more details concerning our semiclassical evaluation of the disorder correlation function, K^d , and corresponding susceptibility $\langle \chi^d(H) \rangle$. We consider non-interacting electrons in a weak, perpendicular magnetic field. In terms of retarded and advanced single particle Green functions, $\mathcal{G}^{+(-)}(\mathbf{r}_1, \mathbf{r}_2; \varepsilon; H)$, K^d may be written as $K^d(\varepsilon_1, \varepsilon_2; H) \approx (\Delta^2/2\pi^2) \mathcal{R} \langle \langle \text{tr } \mathcal{G}^+(\varepsilon_1; H) \text{tr } \mathcal{G}^-(\varepsilon_2; H) \rangle \rangle_d$, where $\langle \langle \dots \rangle \rangle_d$ implies the inclusion of connected diagrams only. Using a diagrammatic approach introduced by Altland and Gefen [3] the field sensitive part of K^d can be expressed as a sum including Cooperon type diagrams $\mathcal{S}_n^{(C)}$ defined by

$$\mathcal{S}_n^{(C)}(\omega; H) = \text{Tr} \left[\zeta^{(C)} \right]^n = \int \prod_{j=1}^n d^d r_j \prod_{m=1}^n \zeta^{(C)}(\mathbf{r}_m, \mathbf{r}_{m+1}; \omega; H) \quad ; \quad \mathbf{r}_{n+1} \equiv \mathbf{r}_1 \quad (2)$$

Here $\zeta^{(C)}(\mathbf{r}_1, \mathbf{r}_2; \omega; H) = (1/2\pi\bar{\nu}\tau) G^+(\mathbf{r}_1, \mathbf{r}_2; \varepsilon_1; H) G^-(\mathbf{r}_1, \mathbf{r}_2; \varepsilon_2; H)$, $G^{+(-)} = \langle \mathcal{G}^{+(-)} \rangle_d$ is the disorder averaged single particle Green function, $\omega = \varepsilon_1 - \varepsilon_2$, and $\tau = \ell/v_F$.

Semiclassically, $G^+(\mathbf{r}_1, \mathbf{r}_2)$ can be expressed as a sum over classical trajectories t between \mathbf{r}_1 and \mathbf{r}_2 [13],

$$G^+(\mathbf{r}_1, \mathbf{r}_2) \simeq \sum_t D_t(\mathbf{r}_1, \mathbf{r}_2) \exp \left[\frac{i}{\hbar} S_t(\mathbf{r}_1, \mathbf{r}_2) - \frac{L_t(\mathbf{r}_1, \mathbf{r}_2)}{2\ell} \right]. \quad (3)$$

The prefactor D_t includes the classical phase space density, S_t stands for the classical action along an orbit t (in the absence of disorder) including the Maslov index, and L_t is the orbit length. $\zeta^{(C)}(\mathbf{r}_1, \mathbf{r}_2; \omega; H)$ is then given in terms of pairs of classical paths which explicitly include the effect of boundary scattering. However most pairs (of different paths) produce oscillating contributions which we assume to vanish after energy or size averaging⁽¹⁾. The main contribution to the field sensitive part of $\langle K^d \rangle_L$ arises from diagonal terms (otherwise known as the Cooperon channel) obtained by pairing paths with their time reverse. Assuming that the magnetic field affects the phase of the particles but not their trajectories we can write $\zeta^{(C)}(\mathbf{r}_1, \mathbf{r}_2; \omega; H) = \sum_{t: \mathbf{r}_1 \rightarrow \mathbf{r}_2} \tilde{\zeta}_t^{(C)}(\mathbf{r}_1, \mathbf{r}_2; \omega; H)$ where

$$\tilde{\zeta}_t^{(C)}(\mathbf{r}_1, \mathbf{r}_2; \omega; H) \simeq \frac{v_F |D_t|^2}{2\pi \bar{\nu} \ell} \exp \left[-\frac{L_t}{L_\phi} - \frac{L_t}{\ell} + i\omega T_t + i\frac{4\pi}{\varphi_0} \int_{\mathbf{r}_1}^{\mathbf{r}_2} \mathbf{A} \cdot d\mathbf{r} \right]. \quad (4)$$

Here, T_t is the period of the trajectory, \mathbf{A} is the vector potential, $\varphi_0 = hc/e$, and the level broadening was introduced via $\omega \rightarrow \omega + i\gamma$. Eq. (4) depends, besides ℓ , only on the system without disorder and holds for both integrable and chaotic geometries.

The disorder induced contribution to the average susceptibility is given by ($\varphi = HL^2/\varphi_0$):

$$\frac{\langle \chi^d(\varphi) \rangle}{|\chi_L|} \approx -\frac{6}{\pi^2} \frac{\partial^2}{\partial \varphi^2} \sum_{n=1}^{\infty} \frac{1}{n} S_n^{(C)}(0; \varphi), \quad (5)$$

where the bulk Landau susceptibility is $\chi_L = -e^2/24\pi mc^2$ for spinless electrons. In Eq. (5) the $S_n^{(C)}$ are now assumed to contain diagonal terms only and their contributions (Eq. (2)) can be calculated by diagonalising $\zeta^{(C)}$ which in general cannot be done analytically. However we can use the fact that all the variations of $\zeta^{(C)}$ occur on classical lengthscales; rapid oscillations on the scale of λ_F cancel out. It is thus possible to discretise the “classical” operator $\zeta^{(C)}$ on a lattice in space with grid size greater than λ_F . By summing over trajectories between lattice cells one can compute $\zeta^{(C)}$, and thereby $\langle \chi^d(H) \rangle$, efficiently by numerical means[14]⁽²⁾.

The propagator $\zeta^{(C)}$ (above Eq. (4)) is made up of a summation over all diagonal pairs of paths (including boundary scattering) between any two given impurities situated at \mathbf{r}_1 and \mathbf{r}_2 . On taking the trace over n propagators $\zeta^{(C)}$, one sees that the field sensitive part of S_n , Eq. (2), consists of a summation over flux-enclosing closed pairs of paths (in position space) involving n impurities and an arbitrary number of boundary scattering events. However this summation does not include closed pairs of paths which follow periodic orbits of the corresponding clean system. Such paths involve zero momentum transfer between the Green functions at the impurity positions; they actually represent disconnected diagrams which are included in $\langle \chi^L(H) \rangle$ and must not be counted again in the determination of $\langle \chi^d(H) \rangle$. It is the presence of these periodic orbits in the determination of $\langle \chi^L(H) \rangle$ ⁽³⁾ that leads to strong sensitivity with respect to the system geometry [16, 17] (see below).

⁽¹⁾ In a ballistic system additional oscillatory terms will however remain upon pure disorder average for fixed size [3, 14].

⁽²⁾ A similar calculation has been applied to a different “classical” operator, describing interaction effects in ballistic quantum dots, in Ref. [15].

⁽³⁾ A similar sensitivity with respect to the system geometry occurs in interacting ballistic quantum dots due to the presence of off-diagonal periodic orbit terms [15].

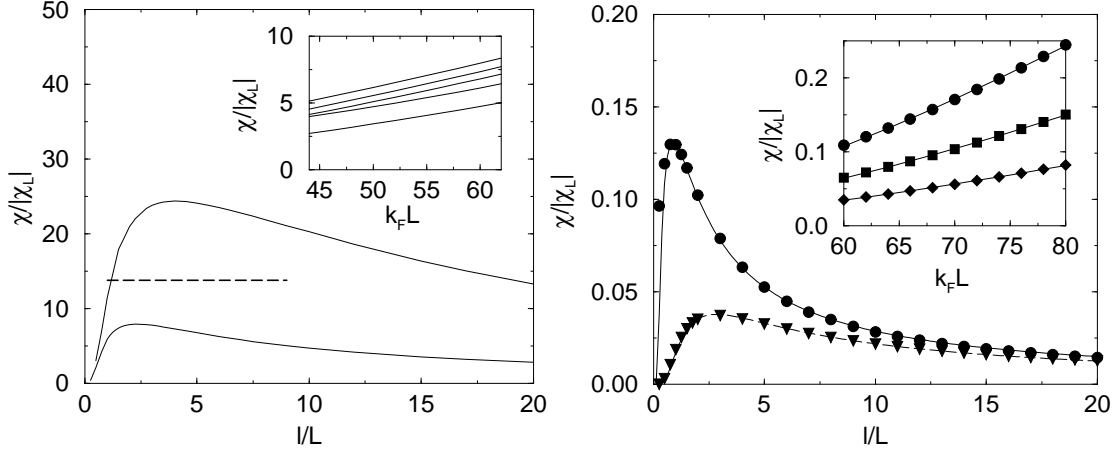


Fig. 1. – Disorder-induced average susceptibility $\langle \chi^d(0) \rangle$ for a square geometry in the elastic regime ($L < \ell < L_\phi$) as a function of the elastic mean free path ℓ for $k_F L = 60$ and two strengths of inelastic scattering, $\gamma/\Delta = 1$ (lower), which corresponds to $L_\phi/L \approx 9.5$, and $\gamma/\Delta = 0.392$ (upper). The dashed horizontal line indicates the result by GBM for $\gamma/\Delta = 1$. The inset shows $\langle \chi^d(0) \rangle$ as a function of $k_F L$ for $\gamma/\Delta = 1$. From the top, the 5 curves are for values of $\ell/L = 2, 4, 5, 1$ and 10 .

Fig. 2. – $\langle \chi^d(0) \rangle$ in the inelastic regime ($L, L_\phi < \ell$) as a function of ℓ for $k_F L = 60$ and $\gamma/\Delta = 10$ which corresponds to $L_\phi/L \approx 0.95$. Circles are our numerical results and the triangles are numerical results including only the contribution of S_1 . The solid and dashed lines are both fits (see main text). The inset shows $\langle \chi^d(0) \rangle$ as a function of $k_F L$ for $\gamma/\Delta = 10$. From the top, the curves are for values of $\ell/L = 2, 4$ and 8 . The symbols correspond to our numerical results and the solid lines to a fit.

In the following we apply the above formalism to the case of an ensemble of disordered square billiards. Gefen, Braun, and Montambaux (GBM) [12] considered the contribution of trajectories longer than ℓ to $\langle \chi^d(H) \rangle$ in an approximate way, while Richter, Ullmo, and Jalabert (RUJ) [13] calculated $\langle \chi^L(H) \rangle$ for a square by assuming that the disorder perturbs the phase, but not the trajectory, of semiclassical paths of the corresponding clean geometry. We first compute the $\mathcal{S}_n^{(C)}$ (Eq. (2)) for the square geometry by employing the extended zone scheme [13] to write $\zeta^{(C)}(\mathbf{r}_1, \mathbf{r}_2; \omega; H)$ as a sum of propagators along straight line paths. We then perform a complete calculation of $\langle \chi^d(H) \rangle$, Eq. (5), in the elastic and inelastic regimes and compare the results with those by GBM and RUJ.

Elastic regime: $L < \ell < L_\phi$. – Fig. 1 shows $\langle \chi^d(0) \rangle$ as a function of ℓ for a typical experimental value of $k_F L = 60$. The lower curve is for $\gamma/\Delta = 1$ (i.e. $L_\phi/L \approx 9.5$ at $k_F L = 60$) and the upper is for $\gamma/\Delta = 0.392$ [18]. Note that in the diffusive regime, $\ell < L$, there is linear increase with ℓ in agreement with Ref. [19]. For $L < \ell < L_\phi$, we find a weak dependence of $\langle \chi^d(0) \rangle$ on ℓ . Our result is on the whole close to the prediction by GBM [12] who found a paramagnetic ℓ -independent contribution, $\langle \chi^d(0) \rangle / |\chi_L| \approx 0.23 k_F L (\Delta/\gamma)$, shown as the dashed horizontal line in Fig. 1 for $\gamma/\Delta = 1$. As ℓ increases further, $\langle \chi^d(0) \rangle$ decreases; we discuss this behaviour in more detail later when considering the inelastic regime.

The inset of Fig. 1 shows $\langle \chi^d(0) \rangle$ as a function of $k_F L$ for $\gamma/\Delta = 1$. From the top, the five curves are for values of $\ell/L = 2, 4, 5, 1$ and 10 . For all disorder strengths, $\langle \chi^d(0) \rangle$ is paramagnetic and it increases linearly with $k_F L$. For $L < \ell < L_\phi$ the gradient of the curves

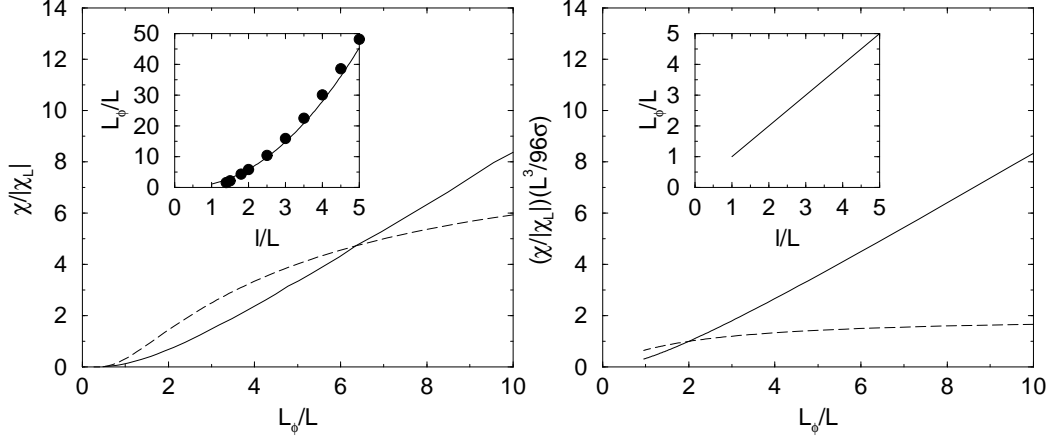


Fig. 3. – Comparison of $\langle \chi^d(0) \rangle$ and $\langle \chi^L(0) \rangle$ for the square. The solid line shows our numerical results for $\langle \chi^d(0) \rangle$ and the dashed line is an analytical expression for $\langle \chi^L(0) \rangle$ (see main text) as a function of L_ϕ/L for $k_F L = 60$ and $\ell/L = 2$. Inset: value of L_ϕ/L at which the two contributions are equal as a function of ℓ/L . The solid line is the analytical estimate Eq. (6) and the circles are obtained by comparing our numerical results for $\langle \chi^d(0) \rangle$ with the analytic expression for $\langle \chi^L(0) \rangle$.

Fig. 4. – Comparison of the (normalized) semiclassical estimates for $\langle \chi^d(0) \rangle$ (solid line) and $\langle \chi^L(0) \rangle$ (dashed) for a generic chaotic geometry for $k_F L = 60$ (see main text). Inset: the (straight) line shows the values in the (ℓ, L_ϕ) -plane where both contributions are equal.

is approximately independent of ℓ and we find it to be $\approx 0.18\Delta/\gamma$. However there is a $k_F L$ independent offset to the curves which is ℓ dependent and not described by GBM.

Inelastic regime: $L, L_\phi < \ell$. – Fig. 2 shows $\langle \chi^d(0) \rangle$ as a function of ℓ for $k_F L = 60$ and $\gamma/\Delta = 10$ (i.e. $L_\phi/L \approx 0.95$). Circular points correspond to our full numerical results, while triangular points represent the contribution of S_1 only (minus the disconnected part) in Eq. (5). The solid line is the equation $\langle \chi^d(0) \rangle = (a_0 L/\ell) \exp(-a_1 L/\ell)$ where a_0 and a_1 are fitting parameters. The dashed line displays an equation of the same type but with $a_1 = 2\sqrt{2}$ and a_0 as the only fitting parameter. For $\ell \gg L$ the susceptibility is dominated by the contribution with the lowest number of impurity scatterings S_1 . As ℓ/L is reduced, progressively more terms in the summation of Eq. (5) become relevant, and there is good agreement with the solid line fit for $\ell \geq L$.

The inset of Fig. 2 shows $\langle \chi^d(0) \rangle$ as a function of $k_F L$ for $\gamma/\Delta = 10$. From the top, the three curves are for values of $\ell/L = 2, 4$ and 8 . The symbols correspond to our results and the solid lines to $\langle \chi^d(0) \rangle = b_0 \exp[-b_1(\gamma/\Delta)/k_F L]$ where b_0 and b_1 are fitting parameters.

Comparison with the contribution of clean correlations. – We compare the magnitude of $\langle \chi^d(0) \rangle$ with that of $\langle \chi^L(0) \rangle$ for squares. It has been shown [16, 17] that the low field susceptibility of an ensemble of *clean* squares is dominated by the shortest flux enclosing periodic orbits of length $L_t = 2\sqrt{2}L$ and their repetitions over a broad range of temperature (and thus inelastic scattering strengths). For the ballistic white noise case considered here, the effect of disorder averaging on the susceptibility was described by an additional damping $\exp(-L_t/\ell)$ of the response of the clean system [13]. This result corresponds to $\langle \chi^L(0) \rangle$ including the disorder damping $\exp(-L_t/2\ell)$ of the single particle Green functions.

We use the results of RUJ [13, 16] at zero temperature and introduce the level broadening γ in the same way as for the disorder correlations above [20]. It is then possible to sum the contribution of all repetitions of the fundamental orbit explicitly which gives $\langle \chi^L(0) \rangle / |\chi_L| \simeq (\sqrt{2}/5\pi) k_F L / \sinh^2[\sqrt{2}(L/\ell + L/L_\phi)]$. Fig. 3 shows this expression for $\langle \chi^L(0) \rangle$ (dashed line) and our numerical results for $\langle \chi^d(0) \rangle$ (solid line) as a function of L_ϕ/L for $k_F L = 60$ and $\ell/L = 2$. Although $\langle \chi^d(0) \rangle < \langle \chi^L(0) \rangle$ for small L_ϕ/L and vice versa for large L_ϕ/L , it is clear that both contributions are relevant over a broad range of L_ϕ/L . We make an estimate for the value of L_ϕ/L at which the contributions of $\langle \chi^L(0) \rangle$ and $\langle \chi^d(0) \rangle$ are equal by comparing the above analytic approximation with that given by GBM. We find for $\ell > L$ that $\langle \chi^d(H) \rangle$ is larger than $\langle \chi^L(H) \rangle$ for L_ϕ greater than a crossover value, L_ϕ^* , given by

$$\frac{L_\phi^*}{L} \sim \frac{(k_F L)^2}{2\pi^2} \left[\sqrt{2} k_F L \left(\frac{L}{\ell} \right)^2 + 8\pi^2 \left(\frac{L}{\ell} \right)^3 \right]^{-1}. \quad (6)$$

The inset of Fig. 3 shows this estimate (solid line) compared to points (circles) obtained by comparing our numerical results for $\langle \chi^d(0) \rangle$ with the analytic expression for $\langle \chi^L(0) \rangle$.

The experiment [11] on the orbital magnetism of ensembles of squares had estimated values for the elastic mean free path of $\ell/L \sim 1-2$, for the phase-coherence length of $\sim (3-10)L$ and for the thermal cutoff length of $L_T/L \sim 2$. Hence, the lengthscale L_ϕ (Eq. (1)) is determined by the shorter length L_T . Fig. 3 shows that for these experimental parameters (and for white noise disorder) both the disorder and size-induced correlations are relevant, however the latter contribution is dominant. The measured value of the susceptibility at *low* temperature was $\chi(0) \sim 100|\chi_L|$, with an uncertainty of about a factor of four. After including a spin factor of 2, the combined contributions $\langle \chi^d \rangle$ and $\langle \chi^L \rangle$ calculated above, together with an interaction contribution of the same order [15], are in broad agreement with the experimental result. We note, however, that a theoretical explanation of the temperature dependence of the measured susceptibility is still lacking.

Experimental ballistic structures as those in Ref. [11] are usually characterised by smooth disorder potentials. The effect of smooth disorder on $\langle \chi^L \rangle$ has been analysed in Ref. [13] showing that the reduction of the clean contribution is less strong than for white noise disorder and no longer exponential. Smooth disorder effects can be incorporated into the present calculation by introducing an angle-dependent cross section for the impurity scattering between two trajectory segments.

Chaotic geometries. – For systems with a generic chaotic, clean counterpart we obtain an analytical estimate for $\langle \chi^d(0) \rangle$ in the elastic regime after transforming the sum over densities $|D_t|^2$ in Eq. (4) into probabilities $P(\mathbf{r}, \mathbf{r}'; t|A)$ to propagate classically from \mathbf{r} to \mathbf{r}' at time t accumulating an “area” A [14]. Assuming a Gaussian “area” distribution with a variance σ , which is taken to be ℓ independent, we find

$$\mathcal{S}_n^{(C)}(\omega; H) \approx \left\{ 1 + \frac{8\pi^2 H^2 \ell \sigma}{\varphi_0^2} + (\gamma - i\omega)\tau \right\}^{-n}. \quad (7)$$

Summation of the $\mathcal{S}_n^{(C)}$, Eq. (5), leads to

$$\frac{\langle \chi^d(0) \rangle}{|\chi_L|} \simeq \frac{96\sigma L_\phi^2}{L^4(L_\phi + \ell)}. \quad (8)$$

$\langle \chi^d(0) \rangle$ is shown as the full line in Fig. 4 which is rather similar to the corresponding curve in Fig. 3 for the square geometry. A corresponding approximation for $\langle \chi^L(0) \rangle$ [17] is shown

as the dashed line in Fig. 4. Both can be shown to add up to an ℓ -independent response $\langle\chi(0)\rangle/|\chi_L| \simeq 96\sigma L_\phi/L^4$ for generic chaotic geometries.

Conclusion. – Disorder-induced spectral correlations and their effect on the magnetic susceptibility in the non-diffusive regime $\ell > L$ were considered. We focused on the square billiard, whose corresponding clean geometry is integrable, and showed that there are two distinct regimes of behaviour depending on the relative magnitudes of ℓ and L_ϕ . This approach enabled us to study the complete crossover from diffusive to clean systems for arbitrary values of ℓ and L_ϕ (smaller than $v_F t_H$). Note that it may be possible to calculate the susceptibility for values of L_ϕ and ℓ greater than $v_F t_H$ using a non-perturbative approach such as the ballistic σ model [21].

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